R & D facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Chemistry and Surface Science

08/2008

Catalysis and Surface Science Facilities

Background

The production of fuels from coal and other fossil resources involves the use of catalysts in several stages of the process. NETL scientists conduct fundamental research on the materials used to produce these catalysts. Data from this research aides in the building of powerful computational models which can guide experimentalists in their development of new catalysts.

From Atoms to Catalysts

At NETL, experimentalists work closely with computational scientists whose atomistic level models help identify new materials for catalyst applications. Fundamental surface science experiments on single-crystals are then conducted to test these models and to provide further data for refinement. Promising systems are scaled up for application scale studies through the synthesis of catalyst powders. A key aspect of this research is NETL's experimental facilities which allow scientists to transition from atomistic level research to lab scale studies of potential catalysts.

State-of-the-Art Facilities

- **Surface Analysis and Imaging System:** NETL has analytical instrumentation that allows for full characterization of the first several atomic layers of a model catalyst system. One instrument houses 6 distinct analytical capabilities and the ability to grow model catalysts in situ. Combining all of these capabilities into one single system allows researchers to study atomically clean surfaces which directly mimic the systems used in computational studies. These experimental capabilities include:
  - Scanning Tunneling Microscopy
  - Atomic Force Microscopy
  - Low Energy Electron Diffraction
  - X-ray Photo Electron Spectroscopy
  - Ion Scattering Spectroscopy
  - Auger Electron Spectroscopy
  - *In Situ* Triple Source E-beam Evaporator

CONTACTS

Charles E. Taylor
Director
Chemistry and Surface Science Division
National Energy Technology Laboratory
626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-6058
charles.taylor@netl.doe.gov

Chris Matranga
Research Group Leader
Chemistry and Surface Science Division
National Energy Technology Laboratory
626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4114
matranga@netl.doe.gov

ADDRESS

National Energy Technology Laboratory
1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

2175 University Avenue South
Suite 201
Fairbanks, AK 99709
907-452-2559

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

One West Third Street,
Suite 1400
Tulsa, OK 74103-3519
918-699-2000

CUSTOMER SERVICE

1-800-553-7681

WEBSITE

www.netl.doe.gov

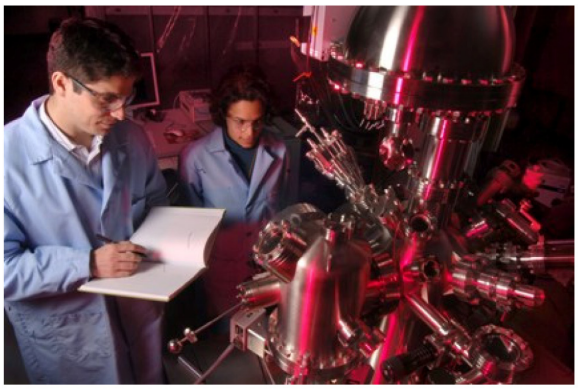
- **In situ Infrared and Raman:** Infrared and Raman spectrometers are coupled to reaction cells for the study of catalyst powders. These cells allow complete control over the temperature, pressure, and gaseous environment the catalyst is exposed to. These systems are used to study fundamental reactions as well as more practical issues related to the conditioning of the catalyst.

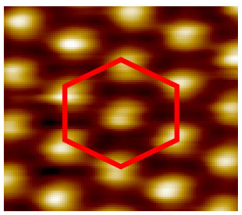
- **X-ray Diffaction:** A PANalytical X-ray Diffraction instrument is equipped with hot and cold stages as well as a high-speed detector. This system allows for the study of structural changes occurring in the catalyst during reactions. Catalyst sintering and other phenomena can also be studied.

- **Chemisorption and Pore Analyzer:** A Quantachrome Autosorb 1C is used for full characterization of the surfaces of a catalyst powder. Temperature programed Reactions (TPR), Temperature Programmed Desorption (TPD), Surface Area Analysis, and adsorption isotherms can be determined.

- **X-ray Photoelectron Spectroscopy with Reaction Cell:** A PHI 5600ci X-ray photoelectron spectrometer is coupled to a reaction cell. Catalysts can be transferred between the spectrometer and reaction cell without exposing the sample to room air. This can allow for identification of intermediate oxidation states and chemical species present during a catalytic reaction.

- **Other Analytical Capabilities** at NETL that are typically utilized for catalyst studies include:
  - Thermogravimetric Analysis
  - Pulse Mass Analyzer
  - Scanning Electron Microscopy
  - Catalytic Reactor Systems





NETL researchers prepare an experiment in the surface analysis and imaging system. These types of experiments result in the atomically resolved image of graphite shown to the right. The hexagonal structure of the surface atoms is apparent. Graphite is a common catalyst support and these substrates serve as model systems for fundamental surface studies.

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